# On restarted Krylov methods for the approximation of matrix functions

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Rolling Waves in Leuven
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## Problem

**Given:**

- $A \in \mathbb{C}^{n \times n}$ large and sparse,
- $\boldsymbol{b} \in \mathbb{C}^n$, $\|\boldsymbol{b}\|_2 = 1$,
- a scalar function $f$.

**Compute** $f(A)\boldsymbol{b}$.

## Problem

**Given:**

- $A \in \mathbb{C}^{n\times n}$ large and sparse,
- $\boldsymbol{b} \in \mathbb{C}^n$, $\|\boldsymbol{b}\|_2 = 1$,
- a scalar function $f$.

**Compute** $f(A)\boldsymbol{b}$.

- $f(z) = z^{-1}$ for solving a linear system of equations,
- $f(z) = \exp(z)$ for the solution of ordinary differential equations,
- $f(z) = \cos(z)$ for certain hyperbolic PDEs,
- $f(z) = \sqrt{z}$ Dirichlet-to-Neumann maps,
- $f(z) = \mathrm{sign}(z)$ in lattice QCD simulations.
- $\ldots$

# Outline

Arnoldi approximation

Restarted Arnoldi approximation

Optimum gradient method

Conjecture

Convergence

Acceleration strategies

# Arnoldi approximation

Extract approximation $\boldsymbol{f}_s$ from Krylov space of order $s$

$$\mathscr{K}_s(A, \boldsymbol{b}) = \mathscr{K}_s = \mathrm{span}\{\boldsymbol{b}, A\boldsymbol{b}, \ldots, A^{s-1}\boldsymbol{b}\}.$$

## Arnoldi method

1. Compute Arnoldi decomposition

$$AV_s = V_s H_s + h_{s+1,s}\boldsymbol{v}_{s+1}\boldsymbol{e}_s^T,$$

   with $V_s = [\boldsymbol{v}_1, \ldots, \boldsymbol{v}_s]$ is ON basis of $\mathscr{K}_s$ and $\boldsymbol{v}_{s+1} \perp \mathscr{K}_s$.
2. Define Arnoldi approximation

$$\boldsymbol{f}_s := V_s f(H_s) V_s^* \boldsymbol{b}.$$

[Druskin & Knizhnerman, 1989], [Gallopoulos & Saad, 1992], ...

## Theorem (Saad, 1992)

*There holds*

$$\boldsymbol{f}_s = V_s f(H_s) V_s^* \boldsymbol{b} = p_{s-1}(A)\boldsymbol{b}$$

*where $p_{s-1}$ is a polynomial of degree $s-1$ which interpolates $f$ at $\Lambda(H_s)$.*

The Arnoldi method can therefore be seen as an interpolation method where the nodes are the eigenvalues of $H_s$ (Ritz values).

## Advantages of Arnoldi method

- avoids $A$ (only $\boldsymbol{v} \to A\boldsymbol{v}$),
- avoids explicit interpolation,
- requires only evaluation of $f(H_s)$ for small matrix $H_s$,
- stable,
- usually good extraction quality (provable for normal $A$).

## Drawbacks

As $s$ gets large,

- size of $V_s$ exceeds computer memory,
- $A$ non-symmetric $\Rightarrow$ orthogonalization cost for $V_s$ grows.

**Cure:** use restarts!

# Restarted Arnoldi approximation

Consider two Arnoldi decompositions

$$\begin{aligned} AV_1 &= V_1 H_1 + h_1 \boldsymbol{v}_1 \boldsymbol{e}_s^T, & \qquad V_1(:,1) &= \boldsymbol{b} \\ AV_2 &= V_2 H_2 + h_2 \boldsymbol{v}_2 \boldsymbol{e}_s^T, & \qquad V_2(:,1) &= \boldsymbol{v}_1. \end{aligned}$$

Glued together they satisfy an Arnoldi-like decomposition

$$A[V_1, V_2] = [V_1, V_2] \begin{bmatrix} H_1 & O \\ E_1 & H_2 \end{bmatrix} + h_2 \boldsymbol{v}_2 \boldsymbol{e}_{2s}^T$$

Shorter:

$$A \hat{V}_2 = \hat{V}_2 \hat{H}_2 + h_2 \boldsymbol{v}_2 \boldsymbol{e}_{2s}^T.$$

The columns of $\hat{V}_2$ are a (non-orthogonal) basis of $\mathscr{K}_{2s}(A, \boldsymbol{b})$.

After $k$ restarts

$$A[\,V_1,\ldots,V_k] = [\,V_1,\ldots,V_k]\begin{bmatrix} H_1 & & & \\ E_1 & H_2 & & \\ & \ddots & \ddots & \\ & & E_{k-1} & H_k \end{bmatrix} + h_k \boldsymbol{v}_k \boldsymbol{e}_{ks}^T$$

Shorter:

$$A\,\hat{V}_k = \hat{V}_k \hat{H}_k + h_k \boldsymbol{v}_k \boldsymbol{e}_{ks}^T.$$

The columns of $\hat{V}_k$ are a (non-orthogonal) basis of $\mathscr{K}_{ks}(A, \boldsymbol{b})$.

Define Arnoldi-like approximation

$$\hat{\boldsymbol{f}}_k := \hat{V}_k f(\hat{H}_k)\boldsymbol{e}_1,$$

then

- there exists an update formula $\hat{\boldsymbol{f}}_{k-1} \longrightarrow \hat{\boldsymbol{f}}_k$ using only $V_k$ and $\hat{H}_k$,
- if $f$ is a rational function in PFE, only $V_k$ and $H_k$ are needed [Afanasjew, Eiermann, Ernst, G., 2008],
- store only $s$ long Krylov basis vectors at a time,
- orthogonalization of less than $s$ vectors per restart.

## Theorem (Eiermann & Ernst, 2006)

*There holds* $\hat{\boldsymbol{f}}_k = p_{ks-1}(A)\boldsymbol{b}$ *where* $p_{ks-1}$ *is a polynomial of degree* $ks-1$ *which interpolates* $f$ *at*

$$\Lambda(\hat{H}_k) = \Lambda(H_1) \cup \Lambda(H_2) \cup \cdots \cup \Lambda(H_k).$$

## Problem

How do these interpolation points behave?

- Since $H_j = V_j^* A V_j$, better look at the blocks $V_j$!

# Optimum gradient method

- For $f(z) = 1/z$ and symmetric positive definite $A$ the restarted Krylov method coincides with the optimum $s$-gradient method.
- For $s = 1$ this is also known as *steepest descend method*.

plied Mathematics vol. 2 (1944) pp. 258–261). Commonly $x_k$ will ultimately behave as though $F(x) = |Ax - b|^2$, where $A$ and $b$ are an appropriate matrix and vector. For $n = 3$ the authors prove that $x_k - x^*$ is asymptotically a linear combination of the eigenvectors belonging to the largest and smallest eigenvalue of $A^T A$ ($A^T$ = transpose of $A$). Furthermore $v_{2k} = \text{grad } F(x_{2k}) / |\text{grad } F(x_{2k})|$ has a limit $v^*$, and $|v_{2k} - v^*| \to 0$ like some $q^k$. (Received January 8, 1951.)

Figure: Abstract by G.E. Forsythe and T.S. Motzkin for a talk on *»Asymptotic properties of the optimum gradient method«* at the 446th meeting of the AMS in New York, 1951.

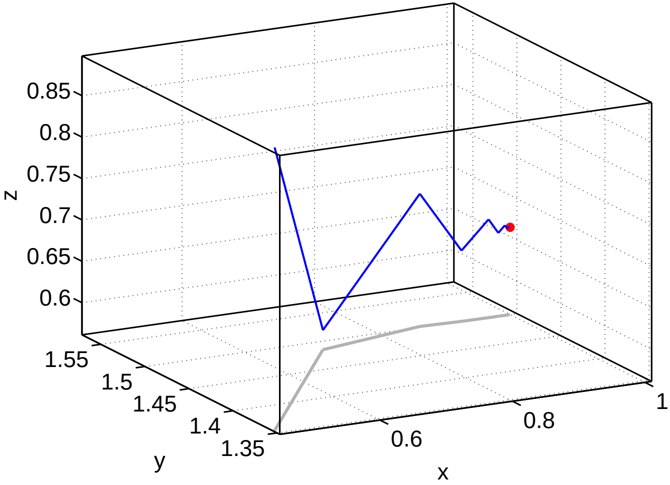



Figure: Iterates of steepest descend for $A = \mathrm{diag}(1,2,3)$ and $\boldsymbol{b} = (1,3,2)^T$

In 1954, Hirotogu Akaike proved in his paper *»On a successive transformation of probability distribution and its application to the analysis of the optimum gradient method«* for arbitrary $n$ and $s = 1$:

**THEOREM 4;** *In the optimum gradient method with respect to the metric* $\|\ \|_P$

i) $\varepsilon_k$ $(=x_k - x)$ *tends to be approximated by a linear combination of two fixed eigenvectors of* $A'PA$ *with the eigenvalues equal to* $\mathrm{Max}\,(\lambda_i\,;(\varepsilon_0,\xi_i)\neq 0)$ *and* $\mathrm{Min}\,(\lambda_i\,;(\varepsilon_0,\xi_i)\neq 0)$, *respectively, and*

ii) $\varepsilon_k$ *alternates asymptotically in two fixed directions.*

In 1968, Forsythe considered the transformation $T$ with

$$V_{k+1}(:,1) = T V_k(:,1) = p_s(A)\, V_k(:,1)$$

and proved

(3.7) **Definition.** By a *continuum* we mean a closed connected set in $E_n$, with the understanding that a single point is a continuum.

(3.8) **Theorem.** *Fix $s$ with $1 \leqq s \leqq n-1$. Let $y_0 = (\eta_1^{(0)}, \ldots, \eta_n^{(0)})^T$ be any vector in $\Sigma^*$ with $\eta_i^{(0)} \neq 0$ $(i = 1, \ldots, n)$. For $k = 0, 1, \ldots,$ define $y_{k+1} = T y_k$, where $T$ was defined in (3.6). Then the set of limit points of the sequence $\{y_{2k}\colon k = 0, 1, 2, \ldots\}$ of normalized gradients is a continuum $R \subset \Sigma^*$. Moreover, for any point $r$ in $R$, we have $r = T^2 r = T(Tr)$.*

Forsythe wrote:

> The author has programmed a number of test cases with $s=2$, to investigate the nature of the set $R$. In every case, $R$ appeared to be a single point. *The author conjectures that $R$ is always a single point in theorem* (3.8). So far, this has been proved only for $s=1$, and we give the proof in (4.12).

If the conjecture is true, then as $k \to \infty$

$$V_k, V_{k+1}, V_{k+2}, V_{k+3}, \ldots = V_a, V_b, V_a, V_b, \ldots.$$

Remember $H_k = V_k^* A V_k$ and therefore

$$H_k, H_{k+1}, H_{k+2}, H_{k+3}, \ldots = H_a, H_b, H_a, H_b, \ldots.$$

In a few slides: The eigenvalues of $H_k$ are interpolation nodes of our restarted Arnoldi method.

# An extended conjecture

Forsythe only considered angles between the first vectors in the block matrices

$$V_k, V_{k+1}, V_{k+2}, V_{k+3}, \ldots$$

(maybe due to memory limitations?)

Nowadays we observe a beautiful symmetry by visualizing the mutual angles between all vectors...

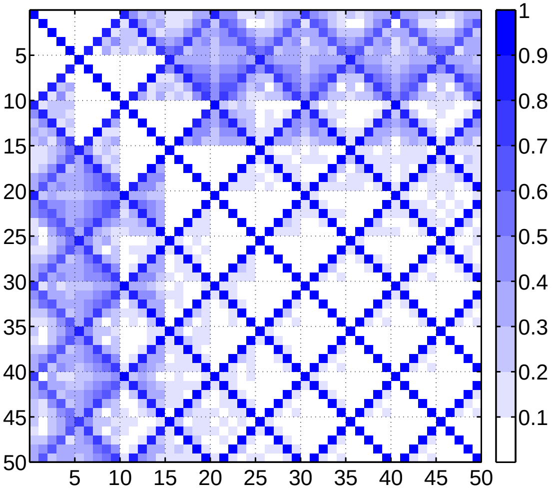



Figure: $s = 5$, each block is entrywise $\sqrt{|\cdot|}$ of $V_j^* V_k$.

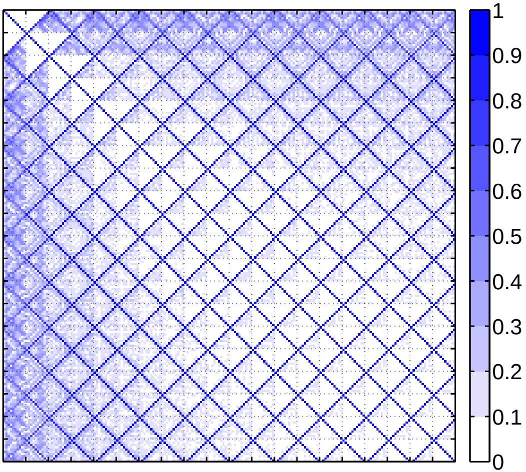



Figure: $s = 10$, each block is entrywise $\sqrt{|\cdot|}$ of $V_j^* V_k$.

## Conjecture

Asymptotically, the normalized directions of the optimum $s$-gradient method are

$$\boldsymbol{y}_1, \boldsymbol{y}_2, \ldots, \boldsymbol{y}_{s-1}, \boldsymbol{y}_s,$$

$$\boldsymbol{y}_{s+1}, \boldsymbol{y}_s, \ldots, \boldsymbol{y}_3, \boldsymbol{y}_2$$

repeated cyclically.

These vectors span an $A$-invariant space of dimension $s+1$.

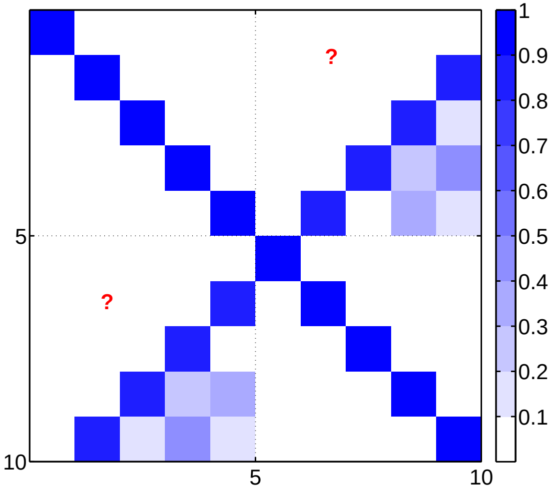



Figure: $s = 5$, zoom in previous picture.

## A strong local version of the conjecture

### Lemma

*Let*

$$\boldsymbol{y}_1, \boldsymbol{y}_2, \ldots, \boldsymbol{y}_s,$$

$$\boldsymbol{y}_{s+1}, \boldsymbol{y}_{s+2}, \ldots, \boldsymbol{y}_{2s}$$

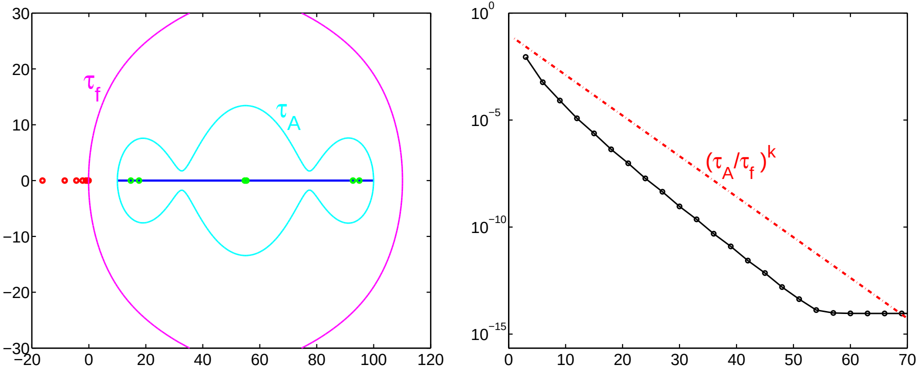
*be the normalized directions produced by 2 consecutive restarts of the optimum $s$-gradient method. Then*

$$\begin{array}{rcll} \boldsymbol{y}_{s+1} & \perp & \boldsymbol{y}_1, \boldsymbol{y}_2, \ldots, \boldsymbol{y}_s & \quad \textit{(by construction)} \\ \boldsymbol{y}_{s+2} & \perp & \boldsymbol{y}_1, \boldsymbol{y}_2, \ldots, \boldsymbol{y}_{s-1} & \\ & \vdots & & \\ \boldsymbol{y}_{2s} & \perp & \boldsymbol{y}_1. & \end{array}$$

# Convergence analysis

Interpolation in cyclically repeated nodes $\vartheta_1, \dots, \vartheta_{2s}$ is well understood:

- look at the level lines $|w(z)| = |(z - \vartheta_1) \cdots (z - \vartheta_{2s})| = \tau^2$.



# Acceleration strategies

Having computed an Arnoldi decomposition

$$AV_1 = V_1 H_1 + h_1 \boldsymbol{v}_1 \boldsymbol{e}_m^T,$$

we can modify it

$$\begin{aligned} AV_1 &= V_1(H_1 - h_1 \boldsymbol{x} \boldsymbol{e}_m^T) + h_1(\boldsymbol{v}_1 + V_1 \boldsymbol{x}) \boldsymbol{e}_m^T \\ &= V_1 \tilde{H}_1 + h_1 \tilde{\boldsymbol{v}}_1 \boldsymbol{e}_m^T. \end{aligned}$$

- The Arnoldi approximation $V_1 f(\tilde{H}_1) V_1^* \boldsymbol{b} = p_{s-1}(A) \boldsymbol{b}$ where $p_{s-1}$ interpolates $f$ at $\Lambda(\tilde{H}_1)$.
- $\Lambda(\tilde{H}_1)$ can be arbitrarily altered with $\boldsymbol{x}$.
- This can be done after each restart.

Thick restarts ([Sorensen, 1992], [Morgan, 2000]) can be applied:

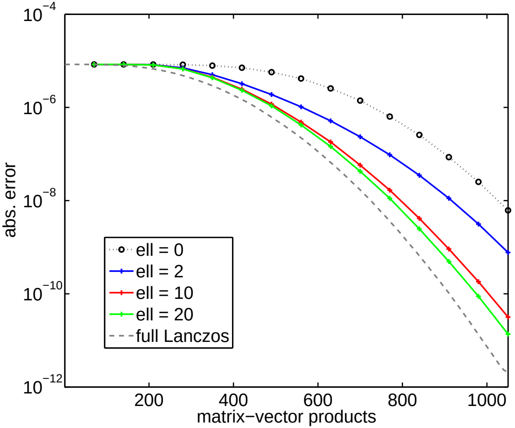



Figure: Solving Maxwell's equation by $\exp(A)\boldsymbol{b}$, $A \in \mathbb{C}^{n\times n}$ symmetric, $n = 565,326$, $s = 70$ [Eiermann, Ernst & G., in prep.].

# Summary

- Restarted Krylov methods are promising if storage is limited.
- Thick-restarts can accelerate the restarted methods.
- (Thick-) restarted Krylov methods are analyzed using Walsh's theory on interpolation polynomials (at least for Hermitian $A$).
- We have extended the Forsythe conjecture.
- For $s = 1$, the Forsythe-Motzkin conjecture can be proven purely algebraic (see [Afanasjew, Eiermann, Ernst & G., 2008]).

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- HAPPY BIRTHDAY to Adhemar!